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Chapter 1

# Spatial Autocatalytic Dynamics: An Approach to Modeling Prebiotic Evolution

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This paper addresses the origin of robust and evolvable metabolic functions, and the conditions under which it took place. We propose that spatial considerations, traditionally ignored, are essential to answering these important questions in prebiotic evolution. Our probabilistic cellular automaton model, based on work on autocatalytic metabolisms by Eigen, Kauffman, and others, has biologically interesting dynamical behavior that is missed if spatial extension is ignored.

## 1.1 Introduction

One difficulty central to any theoretical approach to the study of *prebiotic evolution* is the origin of self-reproduction. Once a reproductive mechanism is in place, the process of mutation and selection of fitter variants acts as feedback that biases the system's parameters towards the direction of improved perfor-

mance. But how is such a mechanism initiated? The difficulty is far from trivial and there is a significant body of research addressing this issue. The central challenge is to understand and describe primitive processes that may have been the precursors of the reproductive and metabolic mechanisms employed by present living systems.

One suggestion is that "the origin of life came about through the evolution of autocatalytic sets of polypeptides and/or single stranded RNA." [8, 10, 11, 9] The central premise is based on the so-called *autocatalytic set*, a set of chemicals in which each member is the product of at least one reaction catalyzed by at least one other member. Such a set allows — in principle at least — for the development of a fortuitous cycle or *catalytic closure*. This mutual support allows the autocatalytic set as a whole to sustain and proliferates at the expense of other species in the chemical soup that do not benefit from such mutual "altruism."

Despite their lack of detail, these models have shown the utility of theoretical approaches to the origin of life. Specifically, they demonstrate that some of the difficulties in making these models work are fundamental ones, and thus likely to be encountered in actual biochemical processes. Two such problems are: i) the problem of generating an evolving chemistry, or more precisely, a chemistry that does not reach fixed points or local minima, and ii) the related problem of understanding how to make such systems responsive to environmental changes.

We argue that the spatial aspect might be an essential ingredient in addressing both problems. Whereas in previous models of autocatalytic sets the underlying assumption was that the chemicals are *perfectly mixed*, here we will allow for *incomplete mixing*. In the context of our model this suggests that chemicals can only interact locally. Our paper is outlined as follows: In Section Two, we give some motivation for the consideration of space in our model, as well as the model specifics. In Section Three, we present some results that show that previous studies on the formation of spiral waves in hypercyclic catalytic sets [4] can be extended to include cross-catalytic reactions. Interestingly, the dynamics of the spatially extended case is qualitatively different from the one observed in the perfectly-mixed case — a situation with no analogue in the previous study based on hypercycles [4]. In Section Four we discuss the potential significance of spatial considerations in the context of the broader research regarding prebiotic evolution.

## 1.2 A model of spatial autocatalytic dynamics

Most of the previous work on autocatalytic sets was formulated and studied in terms of coupled ordinary differential equations. Such formalism implies well-stirred chemostat in which each chemical can interact with every other chemical in the system. Here, we relax the assumption of the perfectly-stirred container. More specifically, we introduce a cellular space in which abstract chemical species can be transported and interact with each other only locally.

The main hypothesis underlying our model is that *spatial organization arising*

*from conditions of incomplete mixing can facilitate chemical organization.* This assertion is encouraged by similar notions of the role of incomplete mixing in related disciplines:

(1) In *population genetics* one school of thought holds that geographical separation speeds up speciation while mixing leads to evolutionary stagnation e.g., [3]. (2) Results in *Artificial Life* literature on modeling ecologies indicate that spatial geometry is conducive to the development of diversity and thus improves the adaptive capabilities of the ecology as a whole [1, 6]. (3) Research in *complex systems*, and *connectionist artificial intelligence* suggests that sparse connectivity (related to the notion of incomplete mixing) is an important ingredient for learning and adaptation [11, 2]. A suggestion arising from this diverse body of work is that sparse connectivity and spatial segregation (incomplete mixing) are important requirements for adaptability and self-organization whereas high-connectivity systems (perfect mixing) have a stronger tendency to move very fast to either an ordered or a chaotic steady state.

### 1.2.1 The Model

We base our model on a probabilistic *cellular automaton* (CA) [13, 15]. Cellular automata are discrete dynamical systems, both in time and in space. An attractive feature of CAs is that typically the update rule of each cellular state depends on a small number of neighboring states — usually its nearest neighbors. This feature enables massively parallel implementations of the CA dynamics.
More specifically, in our CA:

1. The dynamics takes place in a two-dimensional cellular grid.
2. Each cell can either be occupied by a chemical, $I_s$, denoted by a non-zero cellular state, $s$, or empty, denoted by a zero cellular state. We denote the total number of cellular states with $M$.
3. The entire space of cells is permeated by an invisible "ether" from which molecules may be created and into which they may decay. Specifically, the update of the cellular states involves three processes:
   - *Decay.* Occupied states are updated to zero with probability $d$ (see Eq. 2).
   - *Replication.* This process requires an empty cell and one occupied cell in its neighborhood to serve as a replication template [8]. During replication an occupied cell makes a copy of itself, $I_s \xrightarrow{r_s} 2I_s$. $I_s$ denotes the chemical species that undergoes replication and $r_s$ the replication constant.
   - *Auto- and Cross-catalysis.* This process requires an empty cell and two occupied states in its vicinity, one being the template, the other being the catalyst. Figure 1 shows a special case in which the four nearest-neighbor cells can act as template cells and the eight nearest-neighbor cells can act as catalyst cells (for details see figure caption).

4. A *diffusive* process that transports chemicals throughout the system. For simplicity we use the algorithm of Toffoli and Margolus [13] which ensures conservation of chemicals during each diffusion step. To simulate a higher diffusion constant we simply allow more than one diffusion steps.

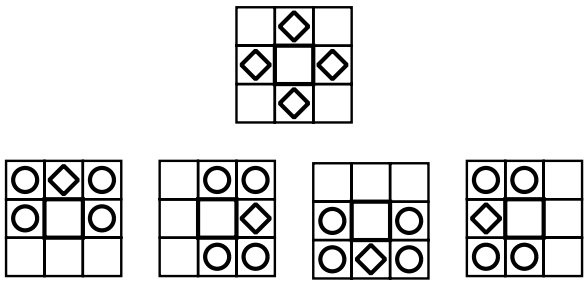

**Figure 1.1**: Example of CA rules required for updating the state of an empty cell (denoted here by the heavy-bordered-square in the center). The state of the empty cell, in the next time step, is determined by the product, $I_{s''}$, of reaction, $I_s + I_{s'} \stackrel{c_{ss's''}}{\rightarrow} I_s + I_{s''} + I_{s'}$ (Eq. (1)). Here, only the four nearest neighbors to the empty cell can serve as a template (diamond-occupied cells in top figure). Furthermore, for every given choice of a template cell, four eligible catalyst cells can be uniquely specified (circle-occupied cells in bottom figures).

Equations 1-3 provide a summary of the probability functions required to update the CA's state. Whenever possible we tried to adhere to the Boerlijst-Hogeweg implementation [4]. Whereas that work focuses on the spatial extension of the hypercycle [8], we are more interested in studying spatial dynamics in autocatalytic sets. Specifically, whereas [4] considered autocatalytic reactions,

$$I_s + I_{s'} \rightarrow 2I_s + I_{s'},$$

where $I_s$ and $I_{s'}$ denote the chemical species serving as template and catalyst respectively, we consider a generalization where the outcome of the templating process, $I_{s''}$, can differ from the chemical species, $I_s$, acting as template,[1]

$$I_s + I_{s'} \stackrel{c_{ss's''}}{\rightarrow} I_s + I_{s''} + I_{s'}, \tag{1}$$

where $c_{ss's''}$ is the catalytic strength for the particular reaction. First we define the probability function $p(i)$, denoting the probability that an occupied site, $i$, remains occupied in the next time step:

$$p(i) = 1 - d, \text{if site i is occupied.} \tag{2}$$

[1] Although from a mathematical point of view the change seems small, it greatly broadens the space of allowed reactions and the resulting dynamics. Such a kind of generalized template replication is also experimentally realizable [12].

Next we define the probability functions $p_s(i), s = 0, \ldots, M$, the probability that an empty site, $i$, will be occupied by chemical $I_s$, or remains empty, in the next time step:

$$p_s(i) = P_s(i) / \sum_{w=0}^{M} P_w(i), s \in \{0, \ldots, M\}, \tag{3}$$

where, $P_0(i) = P_0$, a non-zero constant, allowing for the possibility that an empty site remains empty, and where $P_s$ is defined as follows if $s = 1, \ldots M$,

$$P_s(i) = \sum_{j \in O_i} \delta_{q(j)s} r_{q(j)} + \sum_{w=1}^{M} \sum_{(j,k) \in Q_i} \delta_{ws} c_{q(j)q(k)w}, \tag{4}$$

where we use $q(i)$ to symbolize the cellular state of cell $i$. $O_i$ is the set of four nearest neighbors of cell $i$ that can act as templates. For instance, in the example of Fig. 1, $O_i$ consists of the four sites indicated by $\diamondsuit$ (top part of Fig. 1). $Q_i$ is the set of all template-catalyst pairs of cells in the vicinity of cell $i$. In the example of Fig. 1, $Q_i$ includes all possible $(\diamondsuit, \bigcirc)$ pairs (bottom part of Fig. 1).

## 1.3 Results

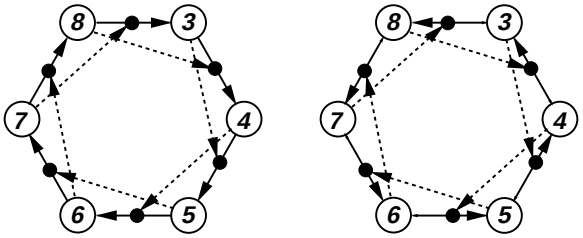


**Figure 1.2**: Chemical Reaction graphs (A) and (B).

Here we are concerned with aspects of the spatial dynamics that are relevant for the study of prebiotic evolution and *cannot* be captured by the perfectly-stirred-container approximation. In that regard a qualification is in order: a broad body of research in pattern formation [5], in general, and in reaction-diffusion systems, in particular, has produced a great variety of spatial dynamics. These studies have clearly demonstrated that the incorporation of space greatly broadens the range of dynamics that can be exhibited by spatially extended systems. However, this new level of complexity might be totally irrelevant to the study of prebiotic evolution if it so happens that the mechanisms of prebiotic processes can be described — at least qualitatively — with models based on the perfectly-stirred-container approximation. In such a case, consideration of imperfect mixing would only improve our understanding of the details rather than of the fundamental underlying mechanisms. Thus, for our approach to be

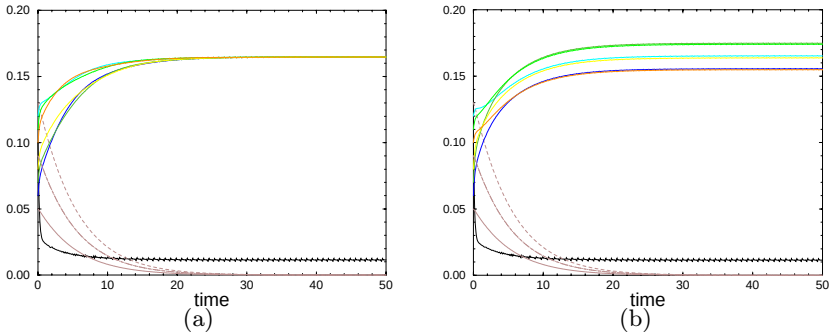


**Figure 1.3**: Perfectly mixed approximation — Evolution of chemical concentrations for two $M = 10$ chemistries (for color code see Fig. caption 5): (a) reaction graph (A); (b) reaction graph (B);

meaningful, it is imperative that it focus on phenomena that i) are essential for the understanding of prebiotic evolution and ii) cannot be studied with the simpler formalism of coupled ordinary differential equations.

We illustrate the point with a simple system of ten ($M = 10$) chemical species. We will consider catalytic reactions of the form, $I_s + I_{s'} \rightarrow I_s + I_{s''} + I_{s'}$ (Eq. 1). In particular, we will focus on two catalytic reaction sets, (A) and (B), graphically depicted in Fig 2. Solid arrows emanate from template chemicals and point to products, while dashed arrows emanate from chemicals that act as catalysts, and point to the reaction that they catalyze. The two graphs are identical except the orientation of the solid arrows. Because we consider a small fraction of all the possible reactions, $c_{ss's''}$, here, is a sparse matrix. For the results reported here we consider a space consisting of size $300 \times 300$ with periodic boundary conditions. Furthermore, we set the model's parameters as follows: $d = 0.2, P_0 = 11, r_s = r = 1, s = 1, \ldots, M$, and all non-zero elements of the catalytic matrix $c_{ss's''}$ to $c = 100$. We have chosen $c$ to be one hundred times larger that $r$ to address the fact that catalytic self-replication is expected to be much more efficient than spontaneous self-replication.

How does such difference in the choice of chemistry affect the resulting dynamics? First we studied the perfectly-mixed case. The results of our numerical simulations are summarized in Figure 3. We note that in both cases the chemical concentrations stabilize to constant values.[2] The situation changes drastically for the imperfectly-mixed case: whereas graph (A) gives rise to dynamics analogous to the ones described above, graph (B) generates a new kind of dynamics (Fig. 4). Now the system has a much higher concentration of empty sites. Furthermore the chemical concentrations follow persistent oscillations where all six chemicals participating in the catalytic set alternate in relative strength (Fig.

[2]More careful study of the dynamics reveals that in chemical graph (A) there is a stronger causal relationship between neighboring reactions (the template of one reaction is also the catalyst of the subsequent reaction) however these differences do not alter the qualitative nature of the overall dynamics.

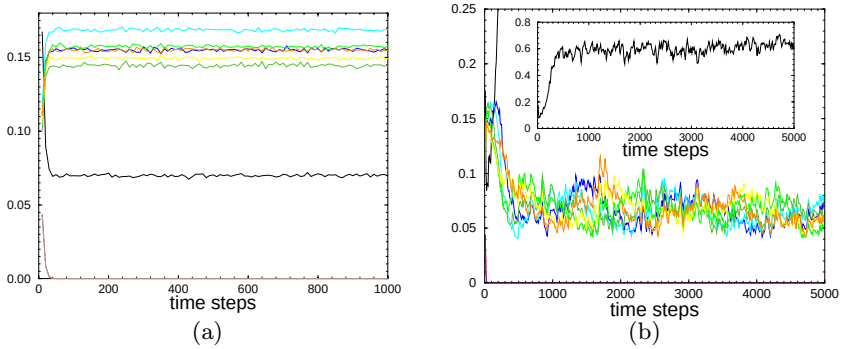


**Figure 1.4**: Imperfectly mixed approximation — Evolution of the chemical concentrations for two 10-chemicals chemistries (for color code see Fig. caption 5): (a) Chemical graph (A); (b) Chemical graph (B) (Inset – concentration of empty sites).

4b). Observation of snapshots of the cellular space (Figs. 5abc) reveals further differences: Case (A) is characterized by fairly homogeneous distribution of the six chemicals participating in the reaction set; very little structure is present in this configuration. Case (B), on the other hand, displays clear signs of spatial self-organization. Fig. 5b displays the state of the system after 1000 time steps; a spatial structure has already started to form. This organization finally leads to the formation of a pair of spiral waves (Fig. 5c). Note the six spiral arms — each color representing a different chemical species — emanating from the spiral center.[3] Further study of a sequence of snapshots of the CA dynamics has shown that the oscillatory pattern of Fig. 4b is directly related to the rotation of the spiral-arm formation. Indeed, the period of the spiral-arm rotation agrees with the period of the oscillation of the chemical concentrations. Finally, it should be noted that for species $I_s$ to receive catalytic support from species $I_{s-2}$ they have to overcome the barrier generated by species $I_{s-1}$. It is the diffusive process, present in the system, that ensures that some of the members of the $I_s$ will eventually be catalyzed by $I_{s-2}$.

The particular reaction graph was chosen i) to demonstrate that spiral dynamics can be extended to autocatalytic sets, and ii) to provide a concrete example of a chemistry whose dynamics cannot be described by the fully-stirred approximation. Furthermore, it suggests that the mechanism underlying the dynamics described above might be extended in situations where the efficient catalytic reactions are relatively few and the ones that lend little or no catalytic support are numerous. In such a system the chemicals forming the autocatalytic set would have to overcome the barrier of a large number of irrelevant chemicals. It would be interesting to know under what conditions — if at all – a diffusive mechanism, similar to the one described above, might allow the members of the autocatalytic set to overcome this barrier.

[3]See ref. [4] for a detailed description of similar spiral dynamics observed in hypercyclic reaction sets.

## 1.4 Discussion

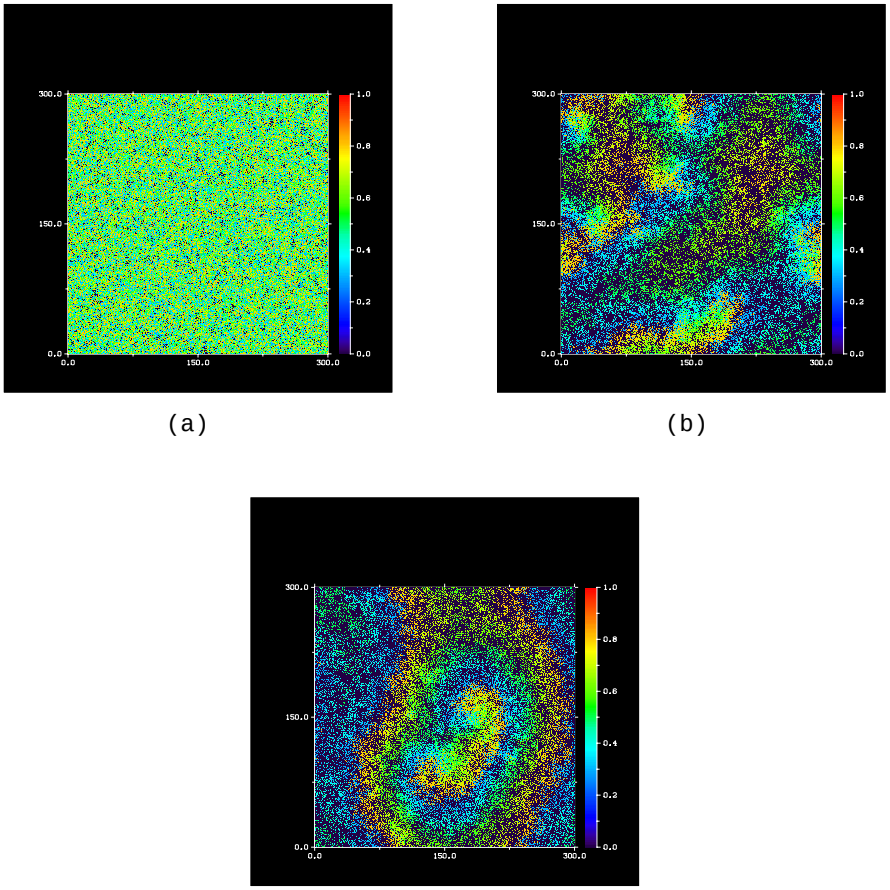


**Figure 1.5**: Snapshots of the CA dynamics; Colors represent different chemicals, (0) black; (3) blue; (4) cyan; (5) green; (6) light green; (7) yellow; (8) orange. (a) reaction graph (A) – system configuration after 1000 time steps; (b) reaction graph (B) – system configuration after 1000 time steps; (c) reaction graph (B) – system configuration after 5000 time steps;

Spiral waves have been previously observed, in the context of prebiotic evolution, in a CA-based model [4] that has added spatial inhomogeneity to the original model on hypercycles [8] by Eigen and co-workers. One aspect of the original work that generated excitement was that in order to proliferate, a hypercycle relies on altruism rather than selectionism. In other words, each member, $I_s$, of the hypercycle lends support to some other member, $I_{s+1}$. From a selectionist perspective this should lead to an increase of species $I_{s+1}$ at the expense

of species $I_s$. In the hypercycle this does not happen because it has been designed so that *every* member lends catalytic support to some other member of the system and at the same time *every* member receives catalytic support.[4] The work in ref. [4] has shown that the same type of mutual interdependence that makes the hypercycle function can be found in the spiral-wave organization found in the extended model. Although that work has shown that the element of space increases the stability of this mechanism (in the sense that spiral-waves seem to be more resilient to parasites) it leaves open the main question namely, "how did a hypercyclic organization come to be in the first place?" We feel that if it can be shown that spiral waves can emerge spontaneously under fairly generic initial conditions, their relevance for modeling prebiotic evolution will deserve serious consideration.

Our work is a first step toward that goal. By opting for a more general catalyzed template reaction (Eq. (1)) we have greatly broadened the space of possible reactions making the accidental occurrence of a hypercycle exceedingly unlikely. Based on a CA-model we have shown that spiral waves are indeed realizable by more general reaction sets. We argue that our choice of set of catalytic reactions is interesting because i) it sustains an organization of mutually dependent species only in the imperfectly-mixed approximation (in the well-stirred case it collapses to a fixed point), and ii) furthermore, the mechanism that generates spiral organizations for this reaction set might also work for more general choices of reaction sets. Ongoing work focuses on a more systematic study of this second point.

## 1.5 Acknowledgments

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